Mixing Properties of Isopropyl Acetate+Aromatic Hydrocarbons at 298.15 K: Density, Refractive Index and Isentropic Compressibility

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Abstract−We present new experimental data of density, refractive index and speed of sound for the binaries of isopropyl acetate+(toluene, ethylbenzene, *p*-xylene, mesitylene, isopropylbenzene, butylbenzene, isobutylbenzene, or *t*-butylbenzene) at T=298.15 K and standard conditions, and the corresponding computed derived magnitudes (change of isentropic compressibility, change of refractive index on mixing, and excess molar volume). The mixtures show a clear expansive tendency for the highest molar weight compounds and the steric hindrance role of the aromatic chemicals being analyzed to the light of the non-ideality on mixing. A good agreement among experimental data and the values estimated by theoretical procedures was obtained.

Key words: Excess Volumes, Change of Refractive Indices, Change of Isentropic Compressibility, Isopropyl Acetate, Aromatic Hydrocarbon, Prediction

INTRODUCTION

Many chemical, food and other industries present non-newtonian and non-ideal fluids and mixtures in their processes. For this reason, it is necessary to pay attention to the thermodynamic rigorous studies and model development to achieve optimal industrial designs. This work is a continuation of a wider project in which the interaction of esters with aromatic hydrocarbons is being investigated. Isopropyl acetate has good solvency characteristics for resins, such as cellulosics, vinyl copolymers, polyesters, polystyrene, acrylics, kauri and manila gums, rosin, dammar, etc. and is commonly used in coatings, cleaning fluids, and as a solvent for fragrances, cosmetics and personal care. One of the main uses is in printing inks where fast evaporation and low hygroscopicity are needed. Other uses include a coalescent in paints, lacquers and coating. Its presence in an aromatic environment is usual and the interactions in mixture are of interest in order to understand and define solubility limits and mechanisms of solvation.

As a continuation of previous works [Resa et al., 1998, 2001, 2002, 2003a, b, c, d], this paper is devoted to the study of different thermodynamic properties of mixtures with chemicals containing the ester group into aromatic environment. To this aim, we present experimental data of the binaries of isopropyl acetate+(toluene, ethylbenzene, *p*-xylene, isopropylbenzene, butylbenzene, isobutylbenzene, mesitylene, or *t*-butylbenzene) measured at standard conditions. The speed of sound, refractive index and density on mixing were measured and then applied to compute the corresponding derived magnitudes, change of isentropic compressibility, change of refractive index on mixing and excess molar volume which were fitted to the Redlich-Kister equation [Redlich and Kister, 1948]. The mixtures show a rising expansive tendency for increasing molar weight

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compounds and the steric hindrance role of the aromatic chemicals being analyzed to explain the non-ideality of mixtures. In what is referred to the as the estimation of these magnitudes, different procedures were applied: Racket [1970] and modified Racket [Spencer and Danner, 1972] equations for density, mixing rules for refractive indices and for isentropic compressibilities, the models of Danusso [1951] and Nomoto [1958], and the Collision Factor Theory (CFT) and Free Length Theory (FLT) theories. As a result, an accurate agreement among the experimental and theoretical values both in magnitude and sign was obtained.

EXPERIMENTAL SECTION

The physical properties of the used chemicals at 298.15 K appear in Table 1 along with other recent literature values. The chemicals were supplied by Fluka, except isopropyl acetate supplied by Panreac, all of them with a purity better than 99.0%. Ultrasonic treatment was used for degassing and also molecular sieves (type 3a, 1/16 inch, Fluka) were introduced into the bottles to reduce possible water content in solvents. The mixtures were prepared by mass using an ER-182A Salter balance with a precision of $\pm 1.0 \times 10^{-4}$ g, special care being taken during solution preparation to avoid evaporation losses. Densities were measured to a precision of $\pm 1.0 \times 10^{-5}$ g·cm^{-3} in an Anton Paar DMA 58 digital vibrating tube densitometer. The apparatus was calibrated periodically, in accordance with technical specifications, using Millipore quality water (resistivity, 18.2 MΩ·cm) and ambient air, as explained in other works [Resa et al., 2003a]. Refractive indices were measured with a precision of $\pm 1.0 \times 10^{-5}$ in a Mettler Toledo RE50 refractometer. An Anton Paar DSA 48 analyzer carried out speed of sound measurements, with a precision of ± 1.0 m·s^{-1} and was also frequently calibrated. Maximum deviation in the calculation of excess molar volumes, changes of refractive indices on mixing, and changes of isentropic compresibilities for these mixtures have been estimated better than

Table 1. Physical properties of the pure solvents at T=298.15 K

Compound	M/g·mol^{-1}	ρ/g·cm^{-3} (Expt)	ρ/g·cm^{-3} (Lit.)^a	n_D (Expt)	n_D (Lit.)^a	u (Expt)	u (Lit.)^b
Isopropyl Acetate	102.133	0.86622	0.8702	1.37460	1.3750	1103.7	1103.7
Toluene	92.14	0.86216	0.86219	1.49400	1.49413	1305.1	1305.0
Ethylbenzene	106.167	0.86273	0.86253	1.49315	1.49320	1319.0	1319.0
p-Xylene	106.167	0.85660	0.85661	1.49308	1.49325	1309.9	1309.7
Mesitylene	120.194	0.86115	0.86111	1.49675	1.49684	1336.6	1336.8
Isopropylbenzene	120.194	0.85757	0.85743	1.48862	1.48890	1307.9	1307.7
Butylbenzene	134.221	0.85615	0.85607	1.48740	1.48742	1331.7	1334.1
Isobutylbenzene	134.221	0.84898	0.84907	1.48393	1.48400	1296.9	1296.9
t-Butylbenzene	134.221	0.86232	0.86240	1.49011	1.49024	1315.4	1315.6

^{a}Organic Solvents [1986].
^{b}Resa et al., 2003.

2.0×10^{-3} cm^3·mol^{-1}, 1.0×10^{-4}, and 1.0 TPa^{-1}, respectively. We are not aware of any such data of these mixtures in previous literature, in the studied conditions.

DATA PROCEDURE

1. Correlation of Derived Magnitudes

The excess molar volumes, changes of refractive indices and changes of isentropic compressibilities on mixing values are presented in Table 2 and were computed from Eqs. (1), (2) and (3):

$$V^E = \sum_{i=1}^{n} x_i M_i (\rho^{-1} - \rho_i^{-1}) \qquad (1)$$

$$\delta n_D = n_D - \sum_{i=1}^{n} x_i n_{Di} \qquad (2)$$

$$\delta \kappa_S = \frac{1}{\rho u^2} - \sum_{i=1}^{n} \frac{x_i}{\rho_i u_i^2} \qquad (3)$$

In these equations, ρ is the density on mixing, n_D the refractive index on mixing and κ_S the isentropic compressibility on mixing. The symbols ρ_i, n_{Di}, u_i and κ_{Si} indicate the properties of pure chemicals and n is the number of components in the mixture. A [Redlich and Kister, 1948] type equation was used to correlate the derived properties of the binary mixtures, by using the unweighted least squares method, all experimental points weighting equally [Marquardt, 1963]. The Redlich-Kister equation can be expressed as:

$$\delta Q = x_i x_j \cdot \sum_{p=0}^{m} B_p (x_i - x_j)^p, \qquad (4)$$

where δQ is V^E/(cm^3·mol^{-1}), δn_D and $\delta \kappa_S$/(TPa^{-1}), respectively. The

Table 2. Thermodynamic properties of isopropyl acetate+(toluene, ethylbenzene, p-xylene, isopropylbenzene, mesitylene, butylbenzene, isobutylbenzene, or t-butylbenzene) at T=298.15 K

			Isopropyl Acetate+Toluene				
x_1	ρ/g·cm^{-3}	V^E/cm^{3}mol^{-1}	n_D	δn_D	u/(ms^{-1})	κ_S/TPa^{-1}	$\delta\kappa_S$/TPa^{-1}
0.0512	0.86262	−0.029	1.48730	−0.0006	1293.9	692.4	−2.2
0.1018	0.86304	−0.054	1.48070	−0.0011	1282.9	704.0	−4.2
0.1500	0.86341	−0.074	1.47447	−0.0016	1272.5	715.3	−5.7
0.1967	0.86374	−0.090	1.46868	−0.0018	1262.5	726.4	−7.1
0.2479	0.86406	−0.104	1.46222	−0.0022	1251.6	738.8	−8.3
0.3056	0.86440	−0.116	1.45504	−0.0025	1239.4	753.2	−9.3
0.3504	0.86463	−0.122	1.44940	−0.0028	1230.0	764.4	−10.0
0.4059	0.86490	−0.128	1.44265	−0.0029	1218.6	778.7	−10.6
0.4498	0.86508	−0.129	1.43733	−0.0030	1209.6	790.1	−10.9
0.5030	0.86528	−0.127	1.43086	−0.0031	1198.8	804.2	−11.0
0.5502	0.86545	−0.125	1.42521	−0.0031	1189.3	816.9	−10.9
0.6009	0.86560	−0.119	1.41933	−0.0029	1179.2	830.8	−10.5
0.6520	0.86574	−0.111	1.41339	−0.0028	1169.2	845.0	−9.9
0.7011	0.86584	−0.099	1.40773	−0.0026	1159.7	858.8	−9.2
0.7488	0.86594	−0.089	1.40230	−0.0023	1150.5	872.4	−8.3
0.8009	0.86603	−0.074	1.39645	−0.0019	1140.6	887.5	−7.1
0.8486	0.86608	−0.057	1.39113	−0.0015	1131.7	901.6	−5.7
0.8990	0.86614	−0.040	1.38561	−0.0010	1122.4	916.5	−4.2
0.9520	0.86618	−0.019	1.37980	−0.0005	1112.6	932.6	−2.4

Table 2. Continued

			Isopropyl Acetate+Ethylbencene				
x_1	ρ/g·cm^{-3}	V^E/cm^{3}mol^{-1}	n_D	δn_D	u/(ms^{-1})	κ_S/TPa^{-1}	$\delta\kappa_S$/TPa^{-1}
0.0489	0.86295	−0.008	1.48759	0.0002	1308.5	676.8	−3.2
0.0998	0.86318	−0.016	1.48176	0.0004	1297.5	688.2	−6.1
0.1494	0.8634	−0.024	1.47606	0.0006	1286.7	699.5	−8.7
0.2013	0.86361	−0.028	1.47026	0.0010	1275.5	711.8	−11.1
0.2488	0.8638	−0.032	1.46459	0.0009	1265.1	723.3	−12.9
0.3018	0.864	−0.035	1.45827	0.0009	1253.7	736.4	−14.8
0.3571	0.8642	−0.036	1.45241	0.0016	1241.6	750.6	−16.1
0.4004	0.86435	−0.036	1.44715	0.0015	1232.3	761.9	−17.0
0.4534	0.86453	−0.036	1.44074	0.0013	1220.8	776.1	−17.7
0.5083	0.86471	−0.034	1.43428	0.0014	1208.9	791.4	−17.9
0.5486	0.86484	−0.032	1.42969	0.0016	1200.2	802.7	−17.9
0.5997	0.865	−0.030	1.42314	0.0011	1189.2	817.5	−17.5
0.6502	0.86515	−0.026	1.417	0.0009	1178.3	832.5	−16.7
0.6993	0.86531	−0.024	1.41128	0.0010	1167.8	847.4	−15.6
0.7504	0.86546	−0.019	1.40548	0.0013	1156.8	863.4	−14.0
0.8010	0.86561	−0.015	1.39903	0.0008	1146.0	879.6	−12.1
0.8499	0.86577	−0.013	1.39314	0.0007	1135.6	895.7	−9.7
0.8999	0.86591	−0.007	1.38692	0.0005	1124.9	912.7	−6.8
0.9513	0.86605	−0.001	1.38054	0.0002	1114.0	930.4	−3.6
			Isopropyl Acetate+p-Xylene				
x_1	ρ/g·cm^{-3}	V^E/cm^{3}mol^{-1}	n_D	δn_D	u/(ms^{-1})	κ_S/TPa^{-1}	$\delta\kappa_S$/TPa^{-1}
0.0487	0.85723	−0.026	1.48765	0.0003	1299.9	690.4	−3.0
0.1006	0.85786	−0.048	1.48187	0.0007	1289.2	701.4	−5.8
0.1463	0.85839	−0.063	1.47679	0.0010	1279.7	711.4	−8.0
0.2006	0.85901	−0.079	1.47055	0.0012	1268.4	723.6	−10.4
0.2499	0.85955	−0.090	1.46526	0.0018	1258.2	734.9	−12.2
0.2997	0.86008	−0.099	1.45933	0.0018	1247.8	746.7	−13.8
0.3508	0.86061	−0.105	1.45324	0.0017	1237.3	759.1	−15.1
0.3983	0.86109	−0.109	1.44775	0.0019	1227.4	770.8	−16.0
0.4546	0.86165	−0.112	1.44093	0.0017	1215.8	785.2	−16.7
0.4970	0.86204	−0.109	1.43621	0.0020	1207.1	796.2	−17.1
0.5498	0.86254	−0.108	1.42975	0.0018	1196.0	810.5	−16.8
0.6021	0.86301	−0.102	1.42335	0.0016	1185.2	824.9	−16.5
0.6533	0.86346	−0.095	1.41719	0.0015	1174.7	839.3	−15.7
0.6967	0.86382	−0.086	1.41203	0.0015	1165.7	851.9	−14.7
0.7470	0.86424	−0.075	1.40588	0.0013	1155.4	866.7	−13.3
0.7998	0.86467	−0.062	1.39955	0.0012	1144.6	882.8	−11.4
0.8511	0.86507	−0.047	1.39315	0.0009	1134.1	898.8	−9.1
0.9007	0.86546	−0.033	1.387	0.0006	1124.0	914.5	−6.6
0.9511	0.86583	−0.014	1.38067	0.0003	1113.8	931.0	−3.6

fitting parameters B_p are gathered into Table 3, with the corresponding root mean square deviations (σ). The root mean square deviations were computed by using Eq. (5), where z is the value of the property, and n_{DAT} is the number of experimental data.

$$\sigma = \left(\frac{\sum_{i=1}^{n_{DAT}} (z_{exp} - z_{pred})^2}{n_{DAT}} \right)^{1/2} \quad (5)$$

In Fig. 1, excess molar volumes are represented as function of composition. The mixtures isopropyl acetate+toluene, ethylbenzene, p-xylene and t-butylbenzene show negative values, isopropylbenzene presents a sigmoid trend (contraction for low compositions of ester), and the others positive values, especially for the mixture with mesitylene. As shown in Fig. 1, these binaries present a rising expansive tendency for the highest molar weight compounds with the steric hindrance role of the aromatic chemicals playing an important role. We can point out the contractive trend for t-butylben-

Table 2. Continued

			Isopropyl Acetate+Mesitylene				
x_1	$\rho/\text{g}\cdot\text{cm}^{-3}$	$V^E/\text{cm}^3\text{mol}^{-1}$	n_D	δn_D	$u/(\text{ms}^{-1})$	κ_S/TPa^{-1}	$\delta\kappa_S/\text{TPa}^{-1}$
0.0509	0.86109	0.045	1.4914	0.0009	1324.7	661.8	−3.4
0.1000	0.861	0.093	1.48599	0.0015	1313.2	673.5	−6.3
0.1538	0.86106	0.121	1.48007	0.0021	1300.6	686.6	−9.2
0.2002	0.86107	0.152	1.475	0.0027	1289.8	698.1	−11.5
0.2575	0.86111	0.185	1.46888	0.0036	1276.3	712.9	−13.8
0.3001	0.86117	0.205	1.46362	0.0035	1266.4	724.1	−15.3
0.3493	0.86126	0.226	1.45786	0.0038	1254.7	737.5	−16.5
0.3994	0.86138	0.242	1.45202	0.0041	1243.2	751.2	−17.7
0.4512	0.86154	0.254	1.44595	0.0043	1230.9	766.2	−18.2
0.4998	0.86172	0.262	1.43996	0.0043	1219.6	780.2	−18.6
0.5518	0.86196	0.263	1.43361	0.0043	1207.5	795.7	−18.5
0.6000	0.86223	0.257	1.42723	0.0038	1196.1	810.6	−18.0
0.6501	0.86252	0.251	1.42132	0.0040	1184.5	826.3	−17.2
0.7000	0.86288	0.236	1.41485	0.0036	1172.9	842.4	−16.0
0.7492	0.86328	0.214	1.40874	0.0035	1161.5	858.7	−14.4
0.8026	0.86376	0.186	1.40156	0.0028	1149.1	876.8	−12.2
0.8497	0.86424	0.155	1.39532	0.0024	1138.3	893.1	−9.9
0.9023	0.86485	0.110	1.38811	0.0016	1126.2	911.7	−6.9
0.9503	0.86548	0.061	1.38157	0.0009	1115.1	929.2	−3.7
			Isopropyl Acetate+Isopropylbenzene				
x_1	$\rho/\text{g}\cdot\text{cm}^{-3}$	$V^E/\text{cm}^3\text{mol}^{-1}$	n_D	δn_D	$u/(\text{ms}^{-1})$	κ_S/TPa^{-1}	$\delta\kappa_S/\text{TPa}^{-1}$
0.0489	0.85795	−0.003	1.48396	0.0009	1298.6	691.1	−3.6
0.0996	0.85835	−0.007	1.47909	0.0018	1289.1	701.1	−7.1
0.1534	0.85878	−0.011	1.47366	0.0025	1278.8	712.1	−10.4
0.2028	0.85917	−0.012	1.46876	0.0033	1269.2	722.5	−13.1
0.2492	0.85954	−0.013	1.46381	0.0036	1260.1	732.7	−15.3
0.2986	0.85994	−0.014	1.45875	0.0042	1250.3	743.9	−17.2
0.3500	0.86034	−0.011	1.45365	0.0049	1240.2	755.8	−19.1
0.4001	0.86075	−0.011	1.44795	0.0050	1230.1	767.8	−20.4
0.4511	0.86116	−0.008	1.4425	0.0053	1219.8	780.4	−21.3
0.5000	0.86156	−0.006	1.4366	0.0050	1209.8	793.0	−21.7
0.5499	0.86197	−0.002	1.43109	0.0052	1199.6	806.2	−21.7
0.6003	0.8624	0.000	1.42477	0.0046	1189.2	820.0	−21.4
0.6511	0.86285	0.001	1.41893	0.0045	1178.6	834.3	−20.6
0.6937	0.86321	0.005	1.4136	0.0041	1169.6	846.8	−19.4
0.7503	0.86372	0.007	1.40687	0.0038	1157.7	863.9	−17.4
0.8003	0.86418	0.009	1.40053	0.0032	1147.0	879.5	−15.1
0.8497	0.86465	0.009	1.39433	0.0026	1136.4	895.5	−12.2
0.9008	0.86516	0.008	1.38776	0.0019	1125.5	912.5	−8.9
0.9506	0.86565	0.009	1.38126	0.0010	1114.6	929.8	−4.8

zene despite its size, perhaps due to the flat structure of the molecule that makes it less bulky and as a consequence does not disrupt the slight polar interactions among ester molecules. In Figs. 2 and 3, changes of refractive index and changes of isentropic compressibility are shown for the studied mixtures. These trends have already been seen in the studied mixtures with other acetates, as shown in earlier works by Resa et al. [1998, 2001, 2002, 2003a, b, c, d] as commented above, being the nature of the ester molecule a determinant factor conditioning these values. We can remark on the huge negative values of the $\delta\kappa_S$, in comparison with those of propyl acetate and butyl acetate, which were also studied by our research team and in the same conditions [Resa et al., 2003a, d]. Such negative values of this derivative magnitude point out the high package capacity of the isopropyl esters around different size of aromatic solvents.

2. Partial Excess Molar Volumes

The expression for the partial excess molar volume should be written as:

Table 2. Continued

Isopropyl Acetate+Butylbenzene							
x_1	ρ/g·cm^{-3}	V^E/cm^{3}mol^{-1}	n_D	δn_D	u/(ms^{-1})	κ_S/TPa^{-1}	$\delta\kappa_S$/TPa^{-1}
0.0492	0.85648	0.009	1.48324	0.0014	1321.8	668.2	−4.6
0.1000	0.85683	0.017	1.47885	0.0027	1311.5	678.5	−9.1
0.1496	0.85719	0.024	1.47432	0.0038	1301.3	688.9	−13.0
0.2005	0.85753	0.038	1.46951	0.0047	1290.6	700.1	−16.5
0.2506	0.85792	0.043	1.46493	0.0058	1280.1	711.3	−19.8
0.2991	0.85832	0.047	1.46025	0.0066	1269.6	722.8	−22.3
0.3507	0.85875	0.052	1.45494	0.0071	1258.5	735.2	−24.8
0.3999	0.85919	0.053	1.45008	0.0078	1247.5	747.9	−26.4
0.4494	0.85964	0.055	1.44452	0.0078	1236.5	760.9	−27.7
0.5022	0.86013	0.058	1.43861	0.0079	1224.4	775.5	−28.3
0.5496	0.86058	0.061	1.43359	0.0082	1213.7	788.8	−28.7
0.6009	0.86113	0.057	1.42758	0.0080	1201.6	804.3	−28.1
0.6496	0.86162	0.060	1.42177	0.0076	1190.1	819.4	−27.0
0.6998	0.8622	0.054	1.41541	0.0069	1178.2	835.6	−25.4
0.7497	0.86278	0.051	1.40937	0.0065	1166.0	852.5	−22.8
0.8009	0.86341	0.045	1.40241	0.0054	1153.2	871.0	−19.2
0.8505	0.86406	0.036	1.39576	0.0043	1140.7	889.4	−15.1
0.9012	0.86475	0.026	1.38897	0.0032	1127.8	909.2	−10.0
0.9496	0.86545	0.015	1.38212	0.0018	1115.3	928.8	−4.3

Isopropyl Acetate+Isobutylbenzene							
x_1	ρ/g·cm^{-3}	V^E/cm^{3}mol^{-1}	n_D	δn_D	u/(ms^{-1})	κ_S/TPa^{-1}	$\delta\kappa_S$/TPa^{-1}
0.0518	0.84963	0.005	1.47964	0.0014	1288.3	709.2	−3.9
0.1011	0.85027	0.008	1.47533	0.0025	1279.9	717.9	−7.4
0.1562	0.851	0.013	1.47075	0.0039	1270.4	728.1	−10.8
0.1994	0.85159	0.016	1.46678	0.0046	1262.8	736.4	−13.2
0.2497	0.8523	0.019	1.46195	0.0053	1253.9	746.3	−15.7
0.3081	0.85314	0.024	1.45684	0.0066	1243.4	758.2	−18.3
0.3497	0.85375	0.028	1.45281	0.0071	1235.8	767.0	−19.8
0.3989	0.8545	0.031	1.44759	0.0073	1226.6	777.8	−21.2
0.4509	0.85531	0.036	1.4424	0.0078	1216.9	789.5	−22.3
0.5015	0.85614	0.037	1.43731	0.0082	1207.1	801.6	−22.8
0.5507	0.85696	0.040	1.43156	0.0078	1197.7	813.5	−23.1
0.6017	0.85785	0.041	1.42563	0.0075	1187.6	826.6	−22.6
0.6503	0.85872	0.042	1.42025	0.0074	1177.9	839.3	−21.8
0.6991	0.85964	0.041	1.41435	0.0069	1168.0	852.8	−20.5
0.7522	0.86066	0.041	1.40776	0.0061	1157.1	867.9	−18.5
0.8030	0.86171	0.035	1.40131	0.0052	1146.3	883.2	−15.7
0.8492	0.86266	0.035	1.39559	0.0045	1136.7	897.2	−13.2
0.9006	0.8638	0.028	1.38855	0.0031	1125.7	913.6	−9.6
0.9488	0.86491	0.020	1.38203	0.0018	1115.2	929.6	−5.4

$$\overline{V}_i^E = (1-x_1)^2\left[\sum_{p=0}^{m} B_p(2x_1-1)^p + x_1\sum_{p=1}^{m}(-2)^{i-1}pB_p(2x_1-1)^{p-1}\right] \qquad (6)$$

where the symbols keep the meaning explained above. From Eq. (6), the corresponding limiting partial excess molar volumes should be determined by considering x_i moles for each case, such limiting values being dependent only on these correlation parameters. In Table 4 the values of limiting partial excess molar volumes at 298.15 K for the binary mixtures are enclosed. These values describe the

solvent behaviour at limit conditions, in what is refered to as accommodation of unlike molecules into bulk solvent at any composition and temperature and show the strong influence of isopropyl acetate into mesitylene liquid phase. Similar behavior for these aromatic chemicals could be observed with the acetate, but attending to structural differences, a decreasing expansive package could be observed as isopropyl acetate abundance is increased at mesitylene mixtures. On the other hand, isopropyl acetate+(p-xylene or toluene) mixtures present a greater tolerance for the inert solvent pres-

Table 2. Continued

				Isopropyl Acetate+*t*-Butylbenzene			
x_1	$\rho/g \cdot cm^{-3}$	V^E/cm^3mol^{-1}	n_D	δn_D	$u/(ms^{-1})$	κ_S/TPa^{-1}	$\delta\kappa_S/TPa^{-1}$
0.0471	0.8625	−0.007	1.48595	0.0013	1306.8	678.9	−4.4
0.0984	0.86271	−0.016	1.4815	0.0028	1297.4	688.6	−8.9
0.1514	0.86293	−0.025	1.47653	0.0039	1287.4	699.2	−13.1
0.1981	0.86312	−0.032	1.47212	0.0049	1278.5	708.8	−16.3
0.2592	0.86336	−0.038	1.46627	0.0061	1266.7	721.9	−20.2
0.3120	0.86355	−0.039	1.46076	0.0067	1256.2	733.8	−23.0
0.3494	0.86371	−0.043	1.45735	0.0076	1248.8	742.4	−24.8
0.3993	0.86391	−0.046	1.45222	0.0082	1238.7	754.4	−26.6
0.4497	0.8641	−0.046	1.44623	0.0081	1228.3	767.0	−28.0
0.5035	0.86429	−0.044	1.44109	0.0091	1217.0	781.2	−28.7
0.5510	0.86448	−0.044	1.43524	0.0088	1206.9	794.2	−28.9
0.6012	0.86468	−0.043	1.4286	0.0079	1196.1	808.4	−28.6
0.6486	0.86485	−0.039	1.42259	0.0074	1185.6	822.5	−27.7
0.6996	0.86503	−0.033	1.41632	0.0070	1174.3	838.4	−26.0
0.7512	0.86521	−0.026	1.41023	0.0069	1162.9	854.7	−24.0
0.8044	0.86541	−0.020	1.40311	0.0059	1150.4	873.1	−20.3
0.8503	0.86559	−0.015	1.39635	0.0045	1139.7	889.4	−16.8
0.9015	0.86579	−0.009	1.38919	0.0032	1127.6	908.4	−12.0
0.9479	0.86597	−0.002	1.38257	0.0019	1116.5	926.4	−6.9

ence (weak polar group, molecular structural similarity), a slight contractive character being observed at any composition (Figs. 4a and 4b), but showing analogous diminution versus composition.

3. Estimation of Physical Properties

Due to strong dependence of design and optimization of chemical processes on computer calculations, the availability of accurate, simple and tested methods, as well as related parameters is of increasing relevance. In this case, consideration was given to the Rackett equation of state [Rackett, 1970; Spencer and Danner, 1972] in order to analyze how accurate densities are predicted. Attending to this model, the density could be described as:

$$\rho = \left(\frac{MP_C}{RT_C}\right) \cdot \beta^{-[1+(1-T_r)^{2/7}]} \tag{7}$$

where T_r is the reduced temperature, T_c and P_c are the critical properties of mixture, M is the average molecular weight in mixture and β is the compressibility factor or an acentric factor dependent parameter which varies attending to a molecular structure parameter [Reid et al., 1988]. The selected mixing rule to compute densities was proposed by Kay (modified combination of Prausnitz-Gunn) [Kay, 1936; Prausnitz and Gunn, 1958]. In order to predict this property, the critical values are required for each compound, open literature or estimative methods being used (as isopropyl acetate, where Joback's method was applied; Poling et al. 2001, or Ambrose method for *t*-butylbenzene, Reid et al., 1987). In Table 6, these critical values are gathered for the compounds enclosed in the studied mixtures. In Table 5, a comparison between the binary experimental and predicted densities is gathered in terms of root mean square deviations, as explained above. In accordance with these results, the following points could be concluded: a) the estimation by modified Rackett equation is closer to the experimental values at all cases, except for isobutylbenzene and b) t-butylbenzene mix-

tures lead to highest deviations.

In what is referred to as refractive indices on mixing, we test the applicability of semiempirical models for refractive index estimation (Lorentz-Lorenz, Dale-Gladstone, Arago-Biot, Eykman, Newton, Oster, Eyring-John, Wiener and Heller [Iglesias et al., 1996]) as a direct tool for predicting. Due to the linear trend of mixing refraction, slight deviations were obtained in the first case as observed in Table 7. For the studied mixtures, accurate results were computed by the Dale-Gladstone and Arago-Biot rules, slight results being obtained by Wiener equation.

For treatment of κ_S values, in the last few years the Collision Factor Theory (CFT) and Free Length Theory (FCT) have proved their applicability for multicomponent estimation and accurate results for mixtures cotaining molecules of different size and nature. Empirical models are also used but their simplicity sometimes leads to poorer results. In this work the empirical models of Danusso and Nomoto are also enclosed [Danusso, 1951; Nomoto, 1958]. Experimental data for the isentropic compressibility of the mixtures were compared with values determined by different mixing procedures. The models of Danusso and Nomoto (Eqs. (8) and (9)) are in accordance with the following expressions:

$$\kappa_S = \left(\frac{1}{M \cdot \rho}\right) \cdot \left(\sum_{i=1}^{N} \frac{n_i M_i}{\rho_i^2 u_i^2}\right) \tag{8}$$

$$\kappa_S = \left(\frac{1}{\rho}\right) \cdot \left(\frac{\sum_{i}^{N} n_i R_i}{\sum_{i}^{N} n_i u_i}\right)^{-6} \tag{9}$$

where $R = u^{1/3} \cdot \sum_{i}^{N} n_i V_i$ and the CFT and FLT [Jacobson, 1952; Nut-

Table 3. Fitting parameters of Eq. (4) and root mean square deviations (σ)

			Isopropyl acetate+Toluene		
$V^E/(cm^3 \cdot mol^{-1})$	$B_0=-0.5118$	$B_1=0.0827$	$B_2=-0.0128$	$B_3=0.0213$	$B_4=0.0169$	$\sigma=4.97 \cdot 10^{-4}$
δn_D	$B_0=-0.0122$	$B_1=-0.0009$	$B_2=0.0013$	$B_3=0.0021$	$B_4=-0.0017$	$\sigma=3.33 \cdot 10^{-5}$
$\delta \kappa_S/(TPa^{-1})$	$B_0=-43.9495$	$B_1=1.0104$	$B_2=0.8735$	$B_3=-2.6916$	$B_4=-6.7544$	$\sigma=4.24 \cdot 10^{-2}$
			Isopropyl acetate+Ethylbenzene		
$V^E/(cm^3 \cdot mol^{-1})$	$B_0=-0.1357$	$B_1=0.0706$	$B_2=-0.0304$	$B_3=-0.0068$	$B_4=0.0654$	$\sigma=6.17 \cdot 10^{-4}$
δn_D	$B_0=0.0056$	$B_1=-0.0013$	$B_2=-0.0013$	$B_3=0.0035$	$B_4=0.0008$	$\sigma=1.60 \cdot 10^{-4}$
$\delta \kappa_S/(TPa^{-1})$	$B_0=-71.7994$	$B_1=-5.3649$	$B_2=-1.7317$	$B_3=0.2863$	$B_4=1.1800$	$\sigma=2.93 \cdot 10^{-2}$
			Isopropyl Acetate+p-Xylene		
$V^E/(cm^3 \cdot mol^{-1})$	$B_0=-0.4410$	$B_1=0.0659$	$B_2=0.0045$	$B_3=0.0673$	$B_4=-0.0135$	$\sigma=6.13 \cdot 10^{-4}$
δn_D	$B_0=0.0072$	$B_1=-0.0022$	$B_2=0.0036$	$B_3=0.0030$	$B_4=-0.0057$	$\sigma=8.93 \cdot 10^{-5}$
$\delta \kappa_S/(TPa^{-1})$	$B_0=-67.8139$	$B_1=-4.8227$	$B_2=2.1355$	$B_3=-1.9628$	$B_4=-6.6139$	$\sigma=3.75 \cdot 10^{-2}$
			Isopropyl Acetate+Mesitylene		
$V^E/(cm^3 \cdot mol^{-1})$	$B_0=1.0448$	$B_1=0.1830$	$B_2=-0.0104$	$B_3=-0.0101$	$B_4=0.1746$	$\sigma=1.81 \cdot 10^{-3}$
δn_D	$B_0=0.0170$	$B_1=-0.0001$	$B_2=0.0028$	$B_3=0.0022$	$B_4=-0.0024$	$\sigma=1.20 \cdot 10^{-4}$
$\delta \kappa_S/(TPa^{-1})$	$B_0=-74.3893$	$B_1=-4.1933$	$B_2=-0.1943$	$B_3=-0.9887$	$B_4=0.8273$	$\sigma=4.90 \cdot 10^{-2}$
			Isopropyl Acetate+Isopropylbenzene		
$V^E/(cm^3 \cdot mol^{-1})$	$B_0=-0.0221$	$B_1=0.0983$	$B_2=-0.0106$	$B_3=0.0280$	$B_4=0.1081$	$\sigma=7.91 \cdot 10^{-4}$
δn_D	$B_0=0.0206$	$B_1=-0.0020$	$B_2=-0.0046$	$B_3=0.0052$	$B_4=0.0065$	$\sigma=1.08 \cdot 10^{-4}$
$\delta \kappa_S/(TPa^{-1})$	$B_0=-86.9650$	$B_1=-10.6610$	$B_2=-0.3873$	$B_3=-2.1944$	$B_4=-3.6479$	$\sigma=4.56 \cdot 10^{-2}$
			Isopropyl Acetate+Butylbenzene		
$V^E/(cm^3 \cdot mol^{-1})$	$B_0=0.2319$	$B_1=0.0431$	$B_2=0.1004$	$B_3=0.0273$	$B_4=-0.1283$	$\sigma=1.36 \cdot 10^{-3}$
δn_D	$B_0=0.0324$	$B_1=0.0029$	$B_2=-0.0016$	$B_3=0.0011$	$B_4=0.0027$	$\sigma=1.02 \cdot 10^{-4}$
$\delta \kappa_S/(TPa^{-1})$	$B_0=-113.3259$	$B_1=-21.1749$	$B_2=-8.9157$	$B_3=22.3455$	$B_4=33.9757$	$\sigma=1.74 \cdot 10^{-2}$
			Isopropyl Acetate+Isobutylbenzene		
$V^E/(cm^3 \cdot mol^{-1})$	$B_0=0.1520$	$B_1=0.0956$	$B_2=-0.0175$	$B_3=0.0683$	$B_4=0.1606$	$\sigma=9.09 \cdot 10^{-4}$
δn_D	$B_0=0.0318$	$B_1=0.0022$	$B_2=-0.0042$	$B_3=0.0037$	$B_4=0.0065$	$\sigma=1.20 \cdot 10^{-4}$
$\delta \kappa_S/(TPa^{-1})$	$B_0=-91.5171$	$B_1=-14.1885$	$B_2=2.4171$	$B_3=-2.4520$	$B_4=-8.7591$	$\sigma=7.40 \cdot 10^{-2}$
			Isopropyl Acetate+t-Butylbenzene		
$V^E/(cm^3 \cdot mol^{-1})$	$B_0=-0.1817$	$B_1=0.0356$	$B_2=0.0297$	$B_3=0.0428$	$B_4=0.0626$	$\sigma=1.03 \cdot 10^{-3}$
δn_D	$B_0=0.0343$	$B_1=0.0019$	$B_2=-0.0071$	$B_3=0.0044$	$B_4=0.0103$	$\sigma=2.50 \cdot 10^{-4}$
$\delta \kappa_S/(TPa^{-1})$	$B_0=-114.9145$	$B_1=-21.2753$	$B_2=-3.6248$	$B_3=-1.5107$	$B_4=-0.5744$	$\sigma=7.97 \cdot 10^{-2}$

sch-kuhnkies, 1965; Schaaffs, 1975]; (Eqs. (10) and (11)) for the isentropic compressibilities were applied:

$$\kappa_S = \left(\frac{1}{\rho^3}\right) \cdot \left(\frac{M}{u_\infty \cdot \sum_i^N x_i S_s \cdot \sum_i^N x_i B_s}\right)^2 \qquad (10)$$

$$\kappa_S = \left(\frac{L_f^2}{K^2}\right) \qquad (11)$$

The CFT is dependent on the collision factors among molecules as a function of temperature into pure solvent or mixture. The pertinent relations in these calculations and its theoretical basis were described in the literature cited. The collision factors (S) and the characteristic molecular volumes (B) of the pure solvents used in the CFT calculations were estimated by using the experimental ultrasonic velocities, included in this paper, and the molar volumes. These values could be also evaluated by means of the group contribution method proposed by Schaaffs [Schaaffs, 1963], when no experimental ones are disposable.

The FLT estimates the isentropic compressibility of a mixture attending to the free displacement of molecules as a main function of temperature. The deviations of each procedure for the studied mixtures are gathered in Table 8 by means of Eq. (5), giving the FLT the better results and Danusso equation the greater deviations in almost all the studied mixtures.

RESULTS AND DISCUSSION

As a continuation of previous works, this paper is devoted to the study of different thermodynamic properties of chemicals containing the ester group into aromatic environment. To this aim, we present experimental data of speed of sound, refractive index on mixing and density for the binaries isopropyl acetate+(toluene, ethylbenzene, p-xylene, mesitylene, isopropylbenzene, butylbenzene, isobutylbenzene, or t-butylbenzene), which were measured and then applied to compute the corresponding derived magnitudes (change of isentropic compressibility, change of refractive index on mixing, and excess molar volume) at T=298.15 K and 1 atm. These mixtures show a rising expansive tendency for the highest molar weigth
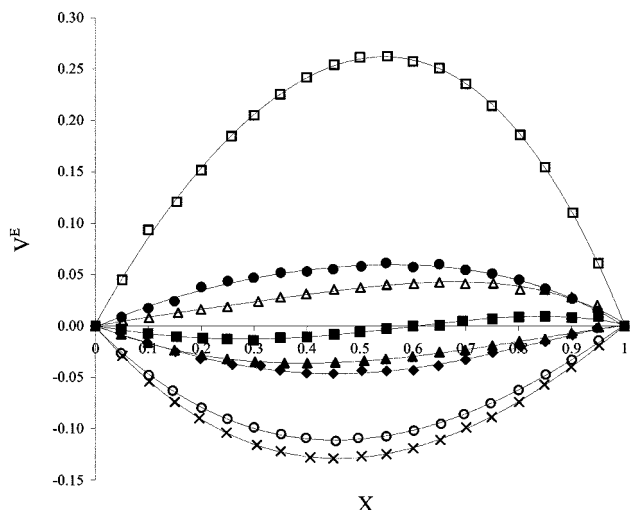
Fig. 1. Dependence of excess molar volumes (cm³·mol⁻¹) with mole fraction at 298.15 K for Isopropyl Acetate+((×) Toluene, (▲) Ethylbenzene, (○) p-Xylene, (□) Mesitylene, (■) Isopropylbenzene, (●) Butylbenzene, (△) Isobutylbenzene or (◆) t-Butylbenzene) and (—) fitting curves.
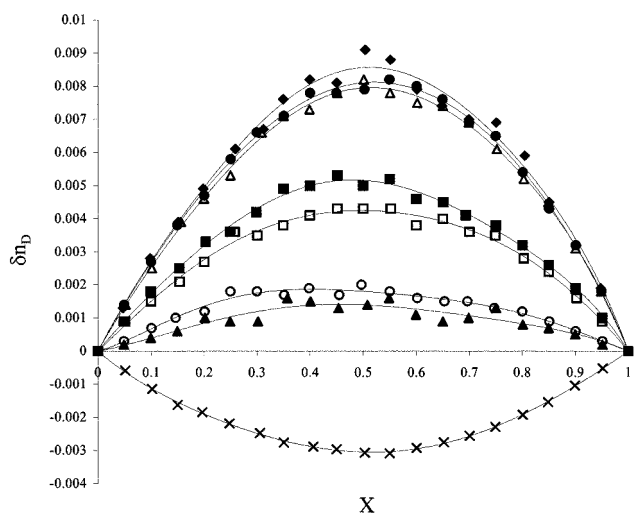

Fig. 2. Dependence of change of refractive index with mole fraction at 298.15 K for Isopropyl Acetate+((×) Toluene, (▲) Ethylbenzene, (○) p-Xylene, (□) Mesitylene, (■) Isopropylbenzene, (●) Butylbenzene, (△) Isobutylbenzene or (◆) t-Butylbenzene) and (—) fitting curves.

compounds, with the steric hindrance role of the aromatic chemicals playing an important role.

In general, the expansibility trend on mixing mainly depends on two effects: a) variation of intermolecular forces when two components come into contact and b) variation of molecular packing as a consequence of differences in the size and shape of the molecules of the components. If the interactions between the molecules of two mixed components are weaker than in the pure component, the excess volume will be positive, as occurs for the highest aromatic molecules. This usually occurs when one of the components has polar groups and the other is a non-polar or weakly polar behavior. Isopropyl acetate is weakly polar and aromatic hydrocarbons are nearly
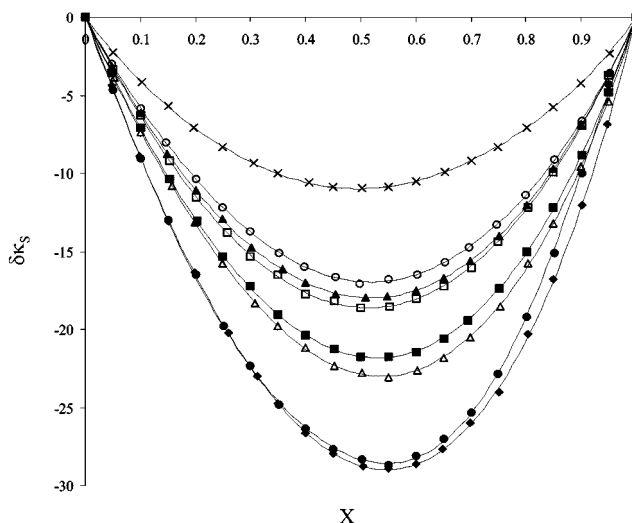
Fig. 3. Dependence of change of isentropic compressibilities (TPa⁻¹) with mole fraction at 298.15 K for Isopropyl Acetate+((×) Toluene, (▲) Ethylbenzene, (○) p-Xylene, (□) Mesitylene, (■) Isopropylbenzene, (●) Butylbenzene, (△) Isobutylbenzene or (◆) t-Butylbenzene) and (—) fitting curves.

Table 4. Partial excess molar volumes at infinite dilution of the binary mixtures isopropyl acetate+aromatic hydrocarbon at 298.15 K

	$\overline{V}_1^{E,\infty}$/(cm³mol⁻¹)	$\overline{V}_2^{E,\infty}$/(cm³mol⁻¹)
Toluene	−0.6117	−0.4037
Ethylbenzene	−0.1645	−0.0369
p-Xylene	−0.5832	−0.3168
Mesitylene	1.0361	1.3819
Isopropylbenzene	−0.0509	0.2017
Butylbenzene	0.0432	0.184
Isobutylbenzene	0.1312	0.459
t-Butylbenzene	−0.1678	−0.011

non-polar. When the pure compounds are mixed, the non-polar hydrocarbon molecules intersperse among the isopropyl acetate molecules, resulting in a decreased interaction among the dipoles of the acetate group. This effect is clearly shown in terms of the partial molar volume at infinite dilution, as commented previously. As polar interactions diminish, the partial excess molar volume becomes positive (infinite dilution) in almost all cases. This causes the differences of the excess volumes from some aromatic hydrocarbons to others. If we compare the maximum excess volumes at equimolar composition, the following observations can be made: negative values correspond to mixtures of flat geometry hydrocarbons with small substituents or separated ones (toluene, p-xylene), intermediate values correspond to mixtures with no-flat geometry hydrocarbons (t-butylbenzene, isopropylbenzene, ethylbenzene) and the highest values correspond to (isopropyl acetate+mesitylene). Mesitylene has a flat geometry and three methyl groups in the meta position around the aromatic ring. The results can be interpreted qualitatively as a consequence of the diminution of the molecular interaction among acetate and aromatic structure due to substituents. The aromatic hydrocarbon molecules will have increasing difficulty in establishing
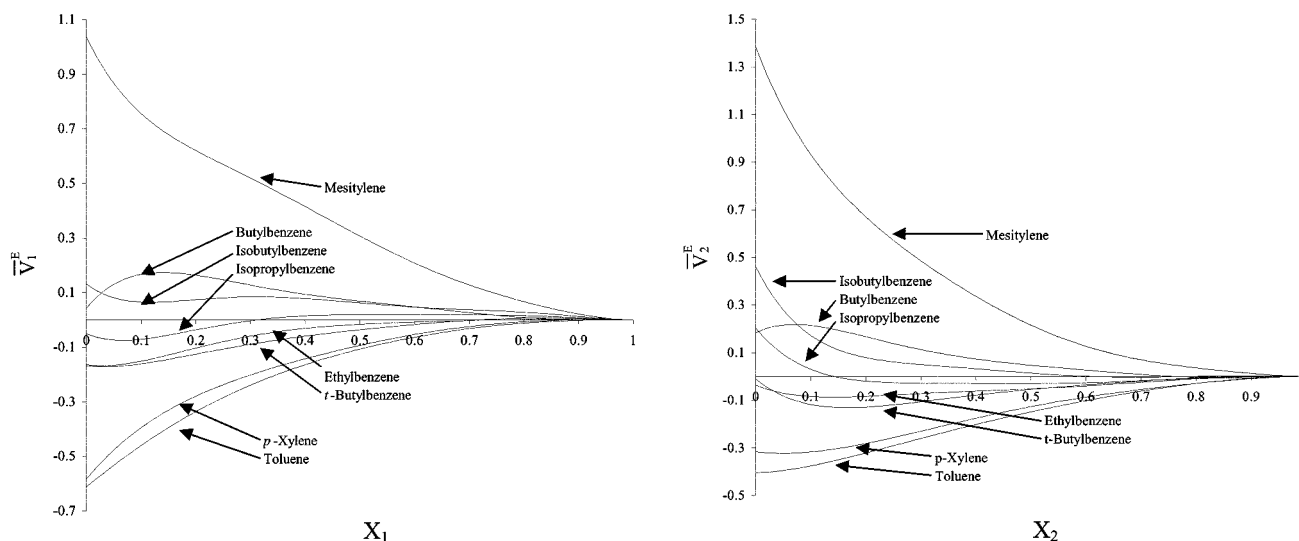
Fig. 4. Partial excess molar volumes (a) $\overline{V}_1^E$ and (b) $\overline{V}_2^E$ of isopropyl acetate+aromatic hydrocarbons as fuction of composition at 298.15 K.

Table 5. Deviations σ (g·cm^{-3}) for predictive density values by rackett (R) or modified rackett (mR) with respect to corresponding experimental data for the binary mixtures isopropyl acetate+aromatic hydrocarbon at 298.15 K

	R	mR
Toluene	0.0320	0.0292
Ethylbenzene	0.0308	0.0235
p-Xylene	0.0291	0.0267
Mesitylene	0.0235	0.0160
Isopropylbenzene	0.0254	0.0177
Butylbenzene	0.0332	0.0124
Isobutylbenzene	0.0266	0.0373
t-Butylbenzene	0.0467	0.0318

interactions the larger they are. If the molecules are flat or with few bulky substituents (toluene, *p*-xylene), some interactions can persist and the excess volume becomes slightly positive, sigmoid or negative. If the hydrocarbon molecules that have bulky substituents are placed in a different plane than the one for the benzenic ring,

the interactions among acetate molecules are disabled and the excess volume will be higher than in the previous case. The presence of three methylene groups in the meta position obstructs the approach of the acetate group towards the ring and the steric volume is higher and the excess volume increases. A similar trend in the excess volume with the size of molecules has been shown in other (non-polar+ polar compounds), such as methyl, ethyl or vinyl acetate with aromatic compounds [Resa et al., 1998, 2001, 2002].

CONCLUSIONS

It is important to point out that as increasing chain in the solvent acetate produces a lower non-ideality on mixing, then higher solvent power could be observed for these kinds of mixtures for non polar substances. The obtained results show the importance of steric hindrance to establish dispersive interactions on mixing and the progressive occultation of the polar effect of ester molecular group, when the chain is increased. Due to the strong dependence of computation and simulation on an adequate industrial design, an estimation of physical properties was made by different theoretical pro-

Table 6. Properties of the pure components used in this study

Compound	P_c (bar)	T_c (K)	V_c (cm^3·mol^{-1})	ω	Z_c	Z_{RA}
Isopropyl acetate*	35.22	531.00	335.5	0.288	0.268	0.265
Toluene	41.08	591.75	316.0	0.264	0.264	0.267
Ethylbenzene	36.09	617.15	374.0	0.304	0.263	0.264
p-Xylene	35.11	616.20	378.0	0.322	0.259	0.262
Mesitylene	31.27	637.30	430.0	0.399	0.252	0.255
Isopropylbenzene	32.09	631.00	434.7	0.326	0.261	0.262
Butylbenzene	28.90	660.50	497.0	0.393	0.262	0.256
Isobutylbenzene	30.50	650.00	480.0	0.383	0.271	0.257
t-Butylbenzene**	29.60	660.00	517.5	0.265	0.270	0.267

Poling et al., 2001.

*V_c and Z_c were estimated by the Joback method [Poling et al., 2001].

**V_c and Z_c were estimated by the Ambrose method [Reid et al., 1987].

Table 7. Root mean square deviations of the experimental refractive indices from the estimation results for the Lorentz-Lorenz (L-L), Dale-Gladstone (D-G), Arago-Biot (A-B), Eykman (Ey), Newton (Nw), Oster (Os), Eyring-Jhon (E-J), Wiener (Wi) and Heller (He) at 298.15 K (non-additivity values marked with asterisk)

L-L	D-G	A-B	Ey	Nw	Os	E-J	Wi	He
			Isopropyl Acetate+Toluene					
0.00089	0.00010	0.00010	0.00023	0.00100	0.00061	0.00040	0.00742	0.00103
*0.00046	*0.00044	*0.00130	*0.00018	*0.00132	*0.00096	*0.00207	*0.00748	*0.00098
			Isopropyl Acetate+Ethylbenzene					
0.00103	0.00018	0.00018	0.00040	0.00086	0.00049	0.00056	0.00752	0.00116
*0.00092	*0.00017	*0.00029	*0.00031	*0.00094	*0.00057	*0.00021	*0.00753	*0.00114
			Isopropyl Acetate+*p*-Xylene					
0.00125	0.00033	0.00033	0.00060	0.00064	0.00027	0.00077	0.00732	0.00138
*0.00090	*0.00012	*0.00069	*0.00029	*0.00088	*0.00053	*0.00121	*0.00736	*0.00134
			Isopropyl Acetate+Mesitylene					
0.00039	0.00065	0.00065	0.00036	0.00162	0.00121	0.00021	0.00881	0.00082
*0.00114	*0.00015	*0.00158	*0.00041	*0.00105	*0.00058	*0.00427	*0.00871	*0.00088
			Isopropyl Acetate+Isopropylbenzene					
0.00099	0.00023	0.00023	0.00042	0.00078	0.00044	0.00056	0.00714	0.00119
*0.00098	*0.00021	*0.00018	*0.00040	*0.00079	*0.00044	*0.00049	*0.00714	*0.00118
			Isopropyl Acetate+Butylbenzene					
0.00091	0.00016	0.00016	0.00034	0.00079	0.00045	0.00049	0.00724	0.00113
*0.00107	*0.00024	*0.00055	*0.00048	*0.00067	*0.00032	*0.00142	*0.00722	*0.00115
			Isopropyl Acetate+Isobutylbenzene					
0.00072	0.00020	0.00020	0.00023	0.00089	0.00057	0.00034	0.00694	0.00094
*0.00083	*0.00017	*0.00028	*0.00030	*0.00081	*0.00048	*0.00095	*0.00693	*0.00095
			Isopropyl Acetate+*t*-Butylbenzene					
0.00126	0.00045	0.00045	0.00068	0.00062	0.00035	0.00082	0.00737	0.00142
*0.00114	*0.00038	*0.00030	*0.00058	*0.00070	*0.00040	*0.00031	*0.00739	*0.00141

Table 8. Root mean square deviations σ (TPa^{-1}) for predicted isentropic compressibilities from experimental data for the binary mixtures isopropyl acetate+aromatic hydrocarbon at 298.15 K

	Nomoto (Eq. (9))	Danusso (Eq. (8))	CFT (Eq. (10))	FLT (Eq. (11))
Toluene	2.69	13.20	5.32	0.36
Ethylbenzene	0.25	10.86	0.43	0.37
p-Xylene	0.14	10.24	1.02	0.33
Mesitylene	6.21	3.17	1.76	0.42
Isopropylbenzene	1.80	7.39	3.71	0.31
Butylbenzene	5.26	5.29	6.23	0.34
Isobutylbenzene	4.26	3.28	6.26	0.25
t-Butylbenzene	3.18	7.12	6.52	0.30

cedures, mainly accurate results being obtained, showing the practical application of the simple models applied.

NOMENCLATURE

B	: molecular volume
B_p	: fitting parameters
L_f	: intermolecular free length
M	: average molecular weight in mixture
M_i	: molar mass of pure component i
n	: number of components in the mixture
n_D	: refractive index on mixing
δn_D	: change of refractive index on mixing
n_{DAT}	: number of experimental data
n_{Di}	: refractive index of pure component i
P_c	: critical pressure of mixture
R	: molar sound velocity
S	: collision factors
T_c	: critical temperature of mixture
T_r	: reduced temperature
u_i	: ultrasonic velocity of pure component i
V_c	: critical volume of mixture
V^E	: excess molar volume on mixing
$\overline{V}_1^E$	: partial excess molar volume of component 1
$\overline{V}_2^E$	: partial excess molar volume of component 2
x_i	: molar fraction of pure component i
x_j	: molar fraction of pure component j

Z_c : compressibility factor
z_{exp} : value of the experimental property
z_{pred} : value of the predicted property
Z_{RA} : compressibility factor that depends on an acentric factor
         parameter

Greek Letters

ω : acentric factor
β : compressibility factor
ρ : density on mixing
ρ_i : density of pure component i
δQ : variation of a magnitude Q
κ_S : isentropic compressibility on mixing
κ_{Si} : isentropic compressibility of pure component i
$\delta \kappa_S$: change of isentropic compressibilities on mixing
σ : root mean square deviation

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